Complex Rheology in a Simple Lattice Gas Model(Mathematical Aspects of Complex Fluids and Their Applications)

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1 Introduction

We investigate the transport behaviors of a simple lattice gas system with a periodic boundary, which consists of only two particles interacting repulsively and the potential forces acting on them. Nonequilibrium lattice gases are simple mathematical models, which have been useful and important in studies of the several properties of nonequilibrium systems with numerous degrees of freedom[1]. Under nonequilibrium conditions, lattice gas systems have been known to show some nontrivial phenomena, such as the appearance of long-range spatial correlations[3] and anomalous drift motions[2], even if the system involves only two particles. In our system, the following novel transport properties are found when only one particle is driven by an external driving field; With the increase in the mean velocity of the driven particle, the coefficient of effective drag of this particle (=[driving field strength]/[mean velocity]) varies in the form, increase → decrease → increase → decrease. Moreover, under other conditions, the coefficient of effective drag shows change similar to that observed in the shear-thickening polymer or colloidal solutions.

2 Model

Now, we introduce a lattice gas model, which is the same as that studied in our previous paper[2]. We consider a lattice system with two parallel one-dimensional lanes where each lane involves L sites with a periodic boundary. Each lane contains only one particle which moves randomly to the nearest sites without changing lanes. The sites occupied by particles in the 1st and 2nd lanes are denoted x_1 and x_2, respectively, which are given as integer numbers from 0 to $L-1$.

The effect of potential forces acting on the particles is described by the following Hamiltonian:

$$H(x_1, x_2) = V(x_1) + V(x_2) + V_{12}(x_1, x_2), \tag{1}$$

where $V(x)$ represents the one-body potential on each lane, and $V_{12}(x_1, x_2)$ represents the interaction potential between the two particles. Furthermore, an external driving field is applied to the particle on the 2nd lane. We denote the field strength F.

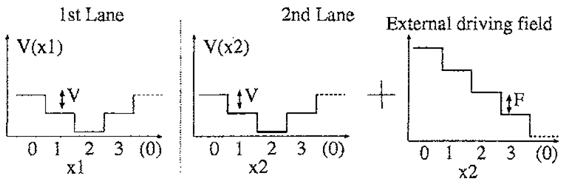

Figure 1: Illustrations of effects of potential and external field in each lane.

The time evolution of this system is described by the iteration of the following three steps. First, one of the two particles is randomly chosen. Let the position of the chosen particle be x. Second, its neighboring site y, $x-1$ or $x+1$, is randomly chosen. Third, the chosen particle moves from x to y with the following probability

$$c(x, y; x_1, x_2) = \frac{1}{1 + \exp[Q(x \to y; x_1, x_2)/k_B T]}, \tag{2}$$

with

$$Q(x \to y; x_1, x_2) = H(x_1', x_2') - H(x_1, x_2) - F(x_2' - x_2), \tag{3}$$

where $(x_1', x_2') = (x_1, y)$ when $x = x_2$, and $(x_1', x_2') = (y, x_2)$ when $x = x_1$. T is temperature and the Boltzmann constant k_B is set 1. Here, the time step is given by [No. of above iterations]/[No. of particles ($= 2$)].

Specifically, we study the case where $V(x) = V|L/2 - x|$ (Fig. 1), and $V_{12}(x_1, x_2) = I\delta_{x_1,x_2}$ using the $L \times L$ unit matrix δ_{ij}. Also, we focus on the case $L = 4$. We found that this size is the minimum required to exhibit the phenomenon we demonstrate in the presented paper.

3 Simulation

Now, we demonstrate a simulation of this system. In particular, we focus on the cases with F as $|F| < I + V$ and T is small enough compared to I and V. Then, the influences of the potential forces and the interactions are strong compared to those of the driving field. In order to characterize the system, we define the mean velocity of the driven particle (in the 2nd lane) in steady state u as the difference of the long time average of the moving ratio in the positive and negative directions. Here, the direction $x_i : 0 \to 1 \to ... \to (L-1) \to 0 \to$ is positive. For simplicity, $I = 1$ and $F > 0$ are set.

Figures 2(a) and (b) show u as a function of F for (a) $V = 0.25$ with $T = 0.05$ or $T = 0.07$ and (b) $V = 0.6$ with $T = 0.08$ or $T = 0.1$. As shown in them, two types of $F - u$ relations, i) u increases steeply with F, ii) u increases slowly with F, appear depending on the range of F. From these results, the relations between u and the coefficient of effective drag of the

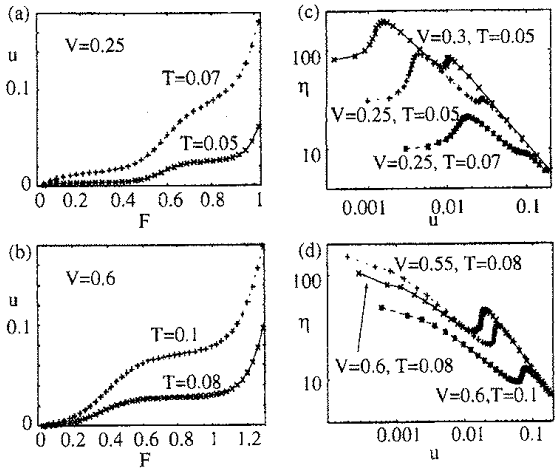

Figure 2: Mean velocity u as a function of F for (a) $V = 0.25$ with $T = 0.05$ or $T = 0.07$ and (b) $V = 0.6$ with $T = 0.08$ or $T = 0.1$, and coefficient of effective drag η as a function of u for (c) $V = 0.25$ or $V = 0.3$ with $T = 0.05$ or $T = 0.07$ and (d) $V = 0.55$ or $V = 0.6$ with $T = 0.08$ or $T = 0.1$.

driven particle η defined as F/u are straightforwardly obtained. Figures 2(c) and (d) show η as a function of u for (c) $V = 0.25$ or $V = 0.3$ with $T = 0.05$ or $T = 0.07$ and (d) $V = 0.55$ or $V = 0.6$ with $T = 0.08$ or $T = 0.1$. As shown in Fig. 2(c), η varies in the form, increase $\rightarrow$ decrease $\rightarrow$ increase $\rightarrow$ decrease, with the increase in u in the case with $V < I/2$ and a small T (for example $V = 0.3$ and $T = 0.05$).

When the smaller V and a little larger T are given (for example, $V = 0.25$ and $T = 0.07$), the change in η becomes less sharp, and simpler in the form, increasing $\rightarrow$ decreasing, with the increase in u (Fig. 2(c)). In this case, the $u - \eta$ profile is given in a form qualitatively similar to that between the shear rate and shear viscosity coefficient of the shear-thickening polymer solutions obtained experimentally[4, 5]. On the other hand, if a larger V is given as in the range $I/2 < V < I$ (for example, $V = 0.55$ and $V = 0.6$), η varies in the form, decrease $\rightarrow$ increase $\rightarrow$ decrease, with the increase in u independently of T (Fig. 2(d)). In this case, the $u - \eta$ profile appears qualitatively similar to that between the shear rate and shear viscosity coefficient of the shear-thickening colloidal solutions obtained experimentally[6].

4 Summary and discussions

In this paper, we investigated the transport behaviors of a simple nonequilibrium lattice gas system. Our results can be easily explained by the considerations of the transition probabilities among (x_1, x_2) ((x_1, x_2): $(0,0) \sim (3,3)$.)[7]. We expect our results to provide important hints to uncover the possible mechanism for several rheological characteristics of several soft materials. Detailed studies for the presented systems should be reported in the other paper in future[7]. Moreover, studies of extended models, including more lanes or particles in the space with more sites or continuous space, and the relations between such toy systems and either real systems or more realistic models of the polymer or colloidal solutions[4, 5, 6] represent important future issues.

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